Methyl formate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 368 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.83e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

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Methoxyethene	N-Methylacetamide	Butylamine
Measured: 586	**Measured:** 216	**Measured:** 245
Predicted: 814	**Predicted:** 6.77e-01	**Predicted:** 107

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4-Methyl-1-pentene	Methoxyacetic acid
Measured: 313	**Measured:** 138
Predicted: 268	**Predicted:** 3.49e-01